WE196 IDENTIFICATION OF UNKNOWNS IN REAL WASTEWATER THROUGH THE APPLICATION OF A LC-QTOF-MS BASED WORKFLOW

P. Gago Ferrero, A. Bletsou, R. Aalizadeh, N.S. Thomaidis, University of Athens / Department of Chemistry. A large number of organic contaminants and related transformation products (TPs) are present in wastewaters. Target analysis methods only allow the detection of a very small fraction of these substances, due to the inability to obtain standards for all that compounds and the ignorance of the existence of many of them. However, advances in high resolution mass spectrometry (HRMS) have opened up new windows of opportunity in the field of complex samples analysis [1]. The application of suspect screening, with suspected substances based on prior information but with no reference standard, greatly increases the list of substances that can be identified. Nevertheless, in most samples there are many peaks in the chromatogram among the most intense ones which not correspond to substances included in the target and suspect screening lists. Therefore, these substances are potentially relevant due to their high concentration and their identification is environmentally important. However, full identification of unknown compounds is often difficult and there is no guarantee of a successful outcome. The aim of this work is to show specific examples on the identification of unknown compounds in real wastewater (collected from the WWTP of Athens). Identifications were conducted using a developed integrated workflow based on liquid chromatography coupled to a quadrupole-time-of-flight mass spectrometer (LC-QToF-MS) to detect suspected and formerly unknown organic contaminants in wastewater. Relevant peaks (not present in our target and suspect lists) were selected based on the intensity and the presence of distinctive isotopic patterns (the most relevant substances with reasonable identification possibilities). For the selected peaks the most plausible molecular formula(s) were determined by applying thresholds of mass accuracy, isotopic pattern and commercial importance. After that, a deep evaluation of the MS/MS spectra was conducted, using both data bases (e.g. Mass Bank) and in silico fragmentation platform (as MetFusion) to find candidates. To assess the plausibility of the candidates a retention time prediction model was also applied. Acknowledgment This project was implemented under the Operational Program «Education and Lifelong Learning» and funded by the European Union (European Social Fund) and National Resources -ARISTEIA 624 (TREMEPOL project). References [1] E. Schymanski et al. Environ Sci Technol 48, 1811 (2014).